Convergence of two-center expansions in positron-hydrogen collisions

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The positron-hydrogen atom scattering system is considered within the S-wave model. Convergence in the elastic scattering, excitation, ionization, and positronium formation channels is studied as a function of the number and type of states used to expand the total wave function. It is found that all unphysical resonances disappear only if near-complete pseudostate expansions are applied to both the atomic and positronium centers.

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In recent years there has been substantial progress in the field of electron-atom collisions. Close-coupling based methods, utilizing near-complete pseudostate expansions about the atomic center, have been shown to yield very accurate results for discrete excitation and ionization channels, see for example [1–4]. This progress is primarily based on the study of the electron-hydrogen atom scattering S-wave model (only states with zero orbital angular momentum are retained) performed by Bray and Stelbovics [5]. They showed, by simply taking a pseudostate expansion whose completeness improves with increasing number of states N, that cross sections for discrete and ionization channels converged at all energies. Pseudoresonances, typically associated with small N calculations, disappeared for sufficiently large N, and convergence was to the correct independently evaluated results. This was an extraordinarily powerful result that is at the base of the substantial success recently enjoyed by the various implementations of the close-coupling theories.

The situation for positron-atom scattering is somewhat more complicated. In addition to the atomically centered states the positronium formation channel needs to be included in the calculations in order to allow for all possible scattering channels. In other words, one needs a combined basis consisting of two independent basis sets. However, in this case if each of the components of the basis is large enough, one may expect instabilities in the calculations. The reason for this is that at small distances between colliding fragments functions of different basis components may essentially repeat each other due to their nonorthogonality. Thus, the close–coupling problem with the combined–basis–expansions

is ill–conditioned. Is this an insurmountable obstacle? This question has remained unanswered for a long time. Mitroy, Berge, and Stelbovics [6] and Mitroy and Ratnavelu [7] have performed convergence studies for the full positron-hydrogen problem at low energies. Below the first hydrogen excitation threshold they showed good agreement between large pseudostate close coupling calculations and the highly accurate variational calculations of Humberston [8]. However, at higher energies, particularly above the ionization threshold the situation is less clear.

We adopt the often-used $CC(N, N')$ notation for close-coupling calculations that utilise N atomic eigenstates and N' positronium eigenstates to expand the total scattering wave function. In addition, a bar, when applied to N or N' indicates that pseudostates rather than eigenstates are used.

In 1991 Higgins and Burke [9] showed that in the close-coupling calculation $CC(1,1)$ a giant resonance appeared around 40 eV incident energy. Since that time a huge body of literature has been devoted to the study of this and other resonances above the ionization threshold, see the excellent review of Walters *et al.* [10]. The positions and widths of the resonances have been studied extensively [11–17], even though, as noted by Walters *et al.* [10], the mid-seventies work of Simon [18,19] shows that there may not be any positron-hydrogen scattering resonances above the ionization threshold.

As far as we are aware the first convincing numerical evidence that shows disappearance of the above-threshold Higgins-Burke type resonances was given by Kernoghan, McAlinden, and Walters [20,21]. They considered the full positron-hydrogen scattering problem using pseudostate expansions on both centers. Their 18-state $CC(\overline{9},\overline{9})$ calculation included s, p, and d states for both centers. Thus it was not clear what was the primary reason, if any, for the disappearance of the Higgins-Burke type resonances. Moreover, at energies above the ionization threshold the authors encountered a new false pseudoresonance structure associated with the unphysical pseudostates. Smooth results for the total and the dominant partial $1s$ cross sections were obtained after applying an energy averaging procedure in order to remove the pseudoresonances. The unsmoothed partial $2s$ and $2p$ cross sections both for atom excitation and positronium formation contained significantly more pseudostructure [22].

At the same time the convergent close-coupling the-

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ory (CCC) [23], which made use of $CC(\overline{N}, 0)$ calculations, i.e. neglected positronium formation, gave very good results for the total, elastic, excitation and ionization cross sections in energy regimes where positronium formation cross section is either zero or small. The CCC calculations showed no pseudoresonances. Based on these results Kernoghan *et al* [22] (see also [24]) suggested using pseudostates only for hydrogen with a few eigenstates of positronium i.e., $CC(\overline{N}, N')$ type calculations. Results of a $CC(\overline{30}, 3)$ calculation with a 30–state hydrogenic pseudobasis of Bray and Stelbovics [23], supplemented by the three lowest positronium eigenstates showed a considerable improvement over the $CC(\overline{9}, \overline{9})$ results [21]. Though the new basis did not completely remove false pseudostructure from the $2s$ and $2p$ positronium formation cross sections in the upper neighbourhood of the ionization threshold, the conclusion was that in two–centre scattering problems $CC(\overline{N}, N')$ type calculations are adequate. Since the works of Kernoghan *et al* [22] and Mitroy [24] pseudostate calculations of positron scattering off atoms have been performed mostly using bases of this type. The same conclusion became dominant in ion-atom collisions as well mainly due to the extensive investigations by Kuang and Lin [25–27].

The purpose of the present Letter is to demonstrate a case where stable and convergent two–centre pseudostate calculations free of any pseudoresonances could be achieved only if near-complete pseudostate expansions are applied to both the atomic and positronium centers, i.e. where calculations of type $CC(\overline{N}, \overline{N'})$ are used. This is done for the simple S-wave model that retains only states of zero orbital angular momentum. The importance of the electron-atom scattering S-wave model, which continues to attract considerable attention [28–30], suggests that this model might also be useful in the positron-hydrogen case. However, for this case it has attracted little attention, with the CC(2,2) calculation by Mitroy [14] being the biggest. Yet, this problem captures most of the difficulties associated with the full positron-atom problem just as the electron-atom S-wave model contains most of the difficulties associated with the full electron-atom scattering problems. At the same time it does not include the unnecessary, in the present context, generalities. Particularly, there is no *a priori* mechanism for any resonances including the Feshbach ones below the ionization threshold, due to the absence of states with non-zero angular momentum. This is why the model is ideal for convergence studies, as only smooth cross sections are expected.

The convergent close-coupling method [1] is extended by including the positronium formation channels. This extension is mainly based on the work of Mitroy [14,31]. However, positronium formation matrix elements have been written as a coupling of 12 j-symbols resulting in only two–dimensional integrals and finite angular momentum sums. In addition, momentum–space pseudostates and corresponding formfactors are used in a compact analytical form. To evaluate the integral over the momentum of the virtual electron involving the logarithmic singularity special–purpose orthonormal polynomials have been calculated which yield an optimal Gaussian quadrature. Together, these features allow big pseudostate calculations to be performed efficiently. The generalized CCC computer code has been tested against the CC(3,3) calculations of Mitroy and Stelbovics [16] and other momentum space close–coupling calculations.

To evaluate the positron-hydrogen S-wave model the total scattering wave function is expanded in terms of bases consisting of two independent truncated Laguerre bases with corresponding exponential fall-off factors λ and λ', leading to close-coupling calculations denoted by $CC(\overline{N}, \overline{N'})$. The $\overline{N}$ hydrogen (H) states were obtained by diagonalising the Hamiltonian with $\lambda \approx 1.0$. The minor variation in λ was made to ensure that the total energy E was exactly half-way between two adjacent pseudothresholds, as the underlying integration rule requires [32,33]. The positronium (Ps) states were obtained by diagonalising the corresponding Hamiltonian with $\lambda' = 0.5$. This choice for λ and λ' results in approximately equal number of negative- and positive-energy states. No variation of λ' was performed due to the fact that at the larger energies (above 40 eV) considered here too large a variation would be necessary to ensure that E is half-way between two adjacent Ps pseudothresholds. Instead, the $CC(\overline{N}, \overline{N'})$ calculations are performed for all possible E that are half-way between two of the Ps pseudothresholds. Though in this case observables are calculated at predefined incident energies, to show convergence in the expected to be smooth cross sections, we combine the results for varying $\overline{N}$ and $\overline{N'}$. If convergence is obtained at the calculated energies such combined results should form smooth curves.

To assure the convergence on both basis components we took $\overline{N} = \overline{N'}$. In general, the combined basis does not need to be symmetric in the number of the hydrogen and positronium pseudostates. The basic momentum space integral equations for the transition matrix elements have been solved using a 96-point Gauss quadrature at each incident energy. The accuracy of the solution of the integral equations has been carefully checked for the case of the largest basis. Any further increase in the number of quadrature points did not significantly change the results. The number of states $\overline{N} = \overline{N'}$ has been systematically increased from 1 to 17.

In Fig. 1 the total cross section for the model is presented evaluated using a number of different bases. The $CC(\overline{N}, N')$ calculations were performed on a fine energy mesh allowing for representation as a continuous curve. The dotted curve labeled CCC is obtained from all of the $CC(\overline{N}, \overline{N'})$ calculations (one for each dot) with $\overline{N} = \overline{N'} = 11, \ldots, 17$, see above. For example, the results at around 114 and 39 eV are from the $CC(\overline{17}, \overline{17})$

calculation and the ones at around 101 and 36 eV are from the CC($\overline{16}, \overline{16}$).
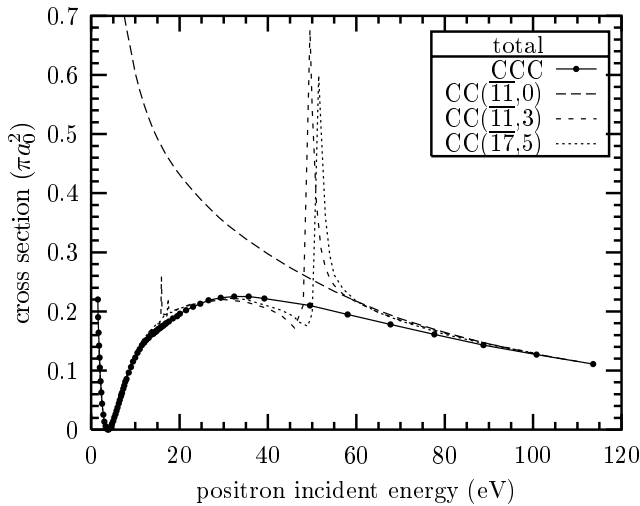

FIG. 1. Total cross section for the positron–hydrogen scattering S–wave model. The CCC-labeled curve is obtained from CC($\overline{N}, \overline{N'}$) calculations with $\overline{N} = \overline{N'} = 11, \ldots, 17$, see text. The CC($\overline{N}, N'$) calculations utilise $\overline{N}$ atomic pseudostates and N' positronium eigenstates.

Starting with the CC($\overline{11}, 0$) calculation we see a smooth cross section that is very large at small energies. Adding three Ps eigenstates ($N' = 3$) results in a massive drop in the cross section at low energies (in fact $N' = 1$ is sufficient for this drop), but leads to Higgins-Burke type resonances at around 15 and 50 eV. Adding a further two Ps eigenstates ($N' = 5$) and increasing the atomic pseudostate expansion to $\overline{N} = 17$ results in only a slight shift of the resonance to higher energies. The shift is due to the increasing number of Ps eigenstates as we found invariance in the CC($\overline{N}, 3$) cross sections for $\overline{N} = 11, \ldots, 17$. However, the CCC curve is smooth devoid of any resonance structure. Thus, within this model the only practical way to yield pseudoresonance-free cross sections is to utilize near-complete pseudostate expansions for both the atomic and Ps centers. We note that the elimination of the Higgins–Burke type resonances is achieved for relatively small $\overline{N} = \overline{N'} = 5$, whereas pseudoresonance structure disappears from $\overline{N} = \overline{N'} = 11$.

Fig. 2 shows some of the individual components of the CCC total cross section given in Fig. 1. The most dominant is the elastic scattering cross section followed by the ionization and Ps formation cross sections. The Ps formation cross section is evaluated by summing the cross sections for the negative-energy Ps states projected onto the Ps true discrete spectrum. The ionization (breakup) cross section is evaluated by subtracting from the total cross section the Ps formation cross section and the sum of the atomic negative-energy state cross sections projected onto the true discrete atomic spectrum. Though the Ps formation cross section is generally very small the

inclusion of the Ps channels considerably reduces the total cross section at energies below 70 eV (see Fig. 1).
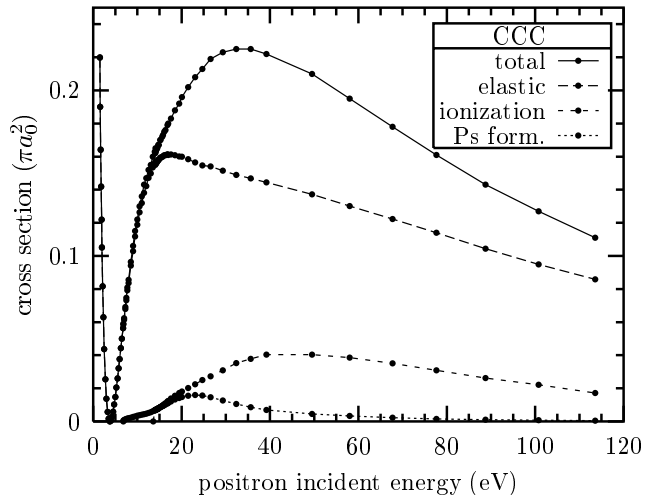

FIG. 2. Total cross section and its components for the S-wave model. See text for the description of the CCC calculations.
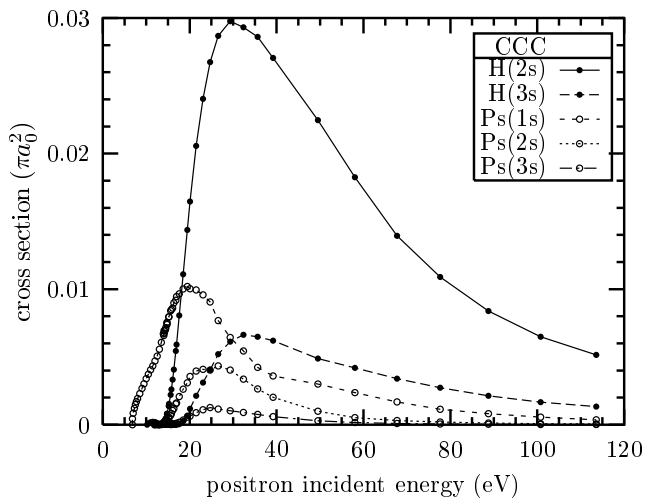

FIG. 3. Discrete H excitation and Ps formation cross sections for $n \leq 3$ states in the S-wave model. See text for the description of the CCC calculations.

The excitation cross sections to $n \leq 3$ are given in Fig. 3. Above the Ps(1s) threshold of 6.8 eV the Ps(1s) cross section is dominant until around 20 eV where H(2s) becomes the largest inelastic cross section. Most importantly we see smooth results for all these cross sections even though their magnitude is quite small. This gives us confidence in the accuracy of the pesented results generally.

In summary, the CCC method for electron-atom scattering [1] has been extended to positron scattering with the inclusion of the Ps formation channel. This channel is particularly important for the S-wave model studied at the low and intermediate energies. Within this model the disappearance of the Higgins–Burke type resonances

is only possible using pseudostate expansions on both the atomic and Ps centers. Other pseudoresonances, resulting from finite pseudostate expansions, disappear if sufficiently large expansions are taken. Utility of using simultaneously two near-complete expansions to yield convergent results at all energies of interest has been demonstrated. Taking as many as 17 of both atomic- and Ps-centered states represents some of the biggest calculations of this type ever performed, and suggests the utility of the present numerical implementation for full positron-atom scattering problems. The presented cross sections represent benchmark results that may be used for comparison with other theories. We suspect that $CC(\overline{N}, \overline{N'})$ type calculations will yield faster convergence and greater accuracy for the full positron-atom scattering system over the commonly-used $CC(\overline{N}, N')$ type calculations, particularly for the Ps formation cross sections.

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